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Supersymmetry, Variational Method and Hulth n Potential

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ABSTRACT

The formalism of Supersymmetric Quantum Mechanics provides us the eigenfunctions to be used in the variational method to obtain the eigenvalues for the Hulth n Potential.

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1 Introduction

The Hulthén Potential, in atomic units, is given by:

$$V_H(r) = -\frac{\delta e^{-\delta r}}{1 - e^{-\delta r}}, \quad (1)$$

where δ is the screening parameter. This potential has been used in several branches of Physics, (see [1] and references therein).

The Schroedinger equation for this potential can be solved in closed form for s waves, [2]. However, for $l \neq 0$ it is necessary to use numerical methods, [1].

Supersymmetric Quantum Mechanics (SQM) has been used to solve Schroedinger equation of solvable potentials, [3], partially solvable ones, [4], in the WKB-approximation, [5], and it has also been applied in variational method, as recently suggested, [6], [7].

The supersymmetric formalism has already been used to study some aspects of the Hulthén potential, [8], [9]. Here, the exact analytical solution for this potential is reobtained, for $l = 0$ to show the consistency of the method. When $l \neq 0$ we interpret that the supersymmetry is “broken” by the potential barrier terms. Nonetheless, the supersymmetry gives us eigenfunctions that allow us to compute the eigenvalues of the variational method. The eigenfunctions for $2p$ and $3d$ states are evaluated for some values of the parameter delta. Our results are compared with direct numerical integration data, [1].

2 The Hulthén Potential with $l = 0$

The Hamiltonian for the Hulthén potential ($l = 0$) can be written as:

$$H_1 = -\frac{1}{2} \frac{d^2}{dr^2} - \frac{\delta e^{-\delta r}}{1 - e^{-\delta r}}. \quad (2)$$

From the Hamiltonian hierarchy we can obtain its eigenfunctions and eigenvalues, [10], [11]. In this way, first we factorise the Hamiltonian (2):

$$H_1 - E_0^{(1)} = a_1^+ a_1^- \quad (3)$$

with creation and annihilation operators defined by

$$a_1^\pm = \frac{1}{\sqrt{2}} (\mp \frac{d}{dr} + W_1(r)) \quad (4)$$

and we determine the ground state eigenvalue $E_0^{(1)}$, the superpotential $W_1(r)$ and the ground state eigenfunction

$$\Psi_0^{(1)} \propto e^{-\int_0^r W_1(r') dr'}. \quad (5)$$

From the operators a_1^+ and a_1^- , we write H_2 , the supersymmetric partner of H_1 as

$$H_2 - E_0^{(1)} = a_1^- a_1^+ \quad (6)$$

and factorise H_2 in an analogous way to (3),

$$a_2^+ a_2^- = H_2 - E_0^{(2)} \quad (7)$$

with a_2^\pm defined similarly to (4). We then determine $E_0^{(2)}$, $W_2(r)$ and $\Psi_0^{(2)}$. Interchanging the operators a_2^+ and a_2^- in (7) we obtain the supersymmetric partner of H_2 . Repeating this process n times we obtain the eigenvalues and eigenfunctions for the n -th ground state Hamiltonian. The superalgebra allows us to relate these results with the original Hamiltonian by the relations:

$$E_n^{(1)} = E_0^{(n+1)}, \quad \Psi_n^{(1)}(r) = a_1^+ a_2^+ \dots a_n^+ \Psi_0^{(n+1)}(r). \quad (8)$$

In our case, using the Hulthén potential, the n -th superpotential is given by

$$W_n(r) = -\frac{n\delta e^{-\delta r}}{1 - e^{-\delta r}} + \frac{1}{n} - \frac{n}{2}\delta \quad (9)$$

that corresponds to the n -th member of the Hamiltonian hierarchy:

$$V_n(r) = W_n^2(r) - \frac{d}{dr}W_n(r) = \frac{n(n-1)\delta^2 e^{-2\delta r}}{2(1 - e^{-\delta r})^2} - \frac{[n(1-n)\delta + 2]\delta e^{-\delta r}}{2(1 - e^{-\delta r})}. \quad (10)$$

The energy-eigenvalue and eigenfunction, eq.(8), are

$$E_n^{(1)} = \frac{1}{2}(-\frac{n}{2}\delta + \frac{1}{n})^2 \quad (11)$$

$$\Psi_0^{(n)}(r) = (1 - e^{-\delta r})^n e^{-[\frac{1}{n} - \frac{n}{2}\delta]r}. \quad (12)$$

We can verify that the energy-eigenvalues (11) are the same given in reference [2].

3 The Hulthén Potential with $l \neq 0$

The Hamiltonian for the Hulthén potential when $l \neq 0$ is written as:

$$H = -\frac{1}{2}\frac{d^2}{dr^2} - \frac{\delta e^{-\delta r}}{1 - e^{-\delta r}} + \frac{l(l+1)}{2r^2}. \quad (13)$$

The potential barrier term prevent us to build the superfamily as in the $l = 0$ case, since the potential is not exactly solvable. However, several numerical approaches have been used in order to evaluate the spectra of energy-eigenvalues and eigenfunctions. In particular, Greene and Aldrich, [12], suggested an Hulthén effective potential in which the eigenfunctions are used as variational trial wave functions.

Based in our results for the case $l = 0$, we introduce a new effective potential whose functional form is suggested by eq.(10),

$$V_{eff}(r) = -\frac{\delta e^{-\delta r}}{1 - e^{-\delta r}} + \frac{l(l+1)}{2} \frac{\delta^2 e^{-2\delta r}}{(1 - e^{-\delta r})^2}. \quad (14)$$

We note that, for small values of δ , the second term of (14) gives us a potential barrier term of (13) in first approximation. This potential differs from the one used in [12] by the exponential numerator which is a quadratic term. The advantage of using the effective potential (14) is the fact that we can vary its parameters without changing its functional form. This is reinforced by the constructive method of determining wave functions based on supersymmetry.

As the effective potential given by (14) has the same functional form as (10), we can solve the Schroedinger problem by the factorisation method of SQM and find the whole super family. The superpotential of the n -th member of the family is given by

$$W_n(r) = B_n \frac{e^{-\delta r}}{1 - e^{-\delta r}} + C_n \quad (15)$$

where

$$B_n = -\frac{1}{2}(\delta + \sqrt{\delta^2 + 4B_{n-1}(B_{n-1} - \delta)}), \quad C_n = -\frac{B_{n-1}(\delta - 2C_{n-1}) - B_n\delta}{2B_n}, \quad (16)$$

and the energy and wave functions are given by (8), where

$$B_1 = -\frac{\delta}{2}(1 + \sqrt{1 + 4l(l+1)}), \quad C_1 = -\frac{\delta}{2} \frac{B_1 + 2}{B_1}, \quad B_0 = 0. \quad (17)$$

The energy eigenvalues and wave functions given by (8) are

$$E_0^{(n+1)} = \frac{1}{2}C_{n+1}^2 \quad (18)$$

$$\Psi_0^{(1)} = (1 - e^{-\delta r})^{-\frac{B_1}{\delta}} e^{-C_1 r}. \quad (19)$$

Notice that B 's and C 's depend on l .

Thus, the spectrum of the effective potential (14) has quantum number $n = 0, 1, \dots$ that shows us which member of the superfamily is going to be used. For instance, $n = 0$ and $l = 1$ corresponds to state $2p$; $n = 1$ and $l = 1$ corresponds to state $3d$ and so on. Fixing $l = 0$ we recover the original Hulthén potential, as expected.

We now look at the Hulthén potential (13) and solve the Schroedinger problem by the variational method. We start from V_{eff} given by (14) whose eigenfunctions are given by (8) and (19). For the state $2p$ we use the first member of the superfamily ($l = 1$) as our trial wave function, changing δ by the variational parameter μ , i.e.,

$$\Psi_\mu = \Psi_0^{(1)}(r, \mu) = (1 - e^{-\mu r})^{-\frac{B_1}{\mu}} e^{-C_1 r}. \quad (20)$$

The energy is obtained by minimisation with respect to μ . Thus, the equation to be minimised is

$$E_\mu = \frac{\int_0^\infty \Psi_\mu(r) \left[-\frac{1}{2} \frac{d^2}{dr^2} - \frac{\delta e^{-\delta r}}{1 - e^{-\delta r}} + \frac{l(l+1)}{2r^2} \right] \Psi_\mu(r) dr}{\int_0^\infty \Psi_\mu(r)^2 dr}. \quad (21)$$

The second derivative in (21) can be evaluated analitically. However, the integration has to be carried out numerically. Our explicit values for the $2p$, ($l = 1$) and $3d$, ($l = 2$) energy states for some values of the parameter δ are listed bellow in Table 1. They are shown together with direct numerical integration data.

Table 1. Energy eigenvalues as a function of the screening parameter for the states $2p$ and $3d$, [eq.(21)]. Comparison is made with numerical data of Ref.[1].

State	Delta	Variational result	Numerical Integration
2p	0.025	-0.112760	-0.1127605
	0.050	-0.101042	-0.1010425
	0.075	-0.089845	-0.0898478
	0.100	-0.079170	-0.0791794
	0.150	-0.059495	-0.0594415
	0.200	-0.041792	-0.0418860
3p	0.025	-0.043601	-0.0437069
	0.050	-0.032748	-0.0331645
	0.075	-0.023010	-0.0239397
	0.100	-0.014433	-0.0160537

4 Conclusions

We have obtained from the formalism of SQM the exact analytical eigenfunction and energy eigenvalue for the Hulthén potential for $l = 0$. When $l \neq 0$, we used an effective potential suggested by the case $l = 0$, to give us a variational trial wave function. The energies for the $2p$ and $3d$ states were obtained for some values of the parameter δ .

We have used the same variational trial wave function for the $2p$ and $3d$ states, eq.(19). The only change was the angular moment number l . However, as the suggested potential has the same functional form, we could determine all the eigenfunctions and therefore we could use the most appropriate in each case, (see [13]).

We note that better results have been obtained for the $2p$ state, for small values of δ . This is expected since for small values of δ the effective potential (14) becomes closer to the original Hulthén potential (13), and for l small the contribution of this angular moment term in the potential is also small. The advantage of this process is that only the form of the potential (14) is important to obtain the eigenfunctions; the multiple parameters can be changed conveniently in order to obtain better results.

The algorithm used here is very powerful because it gives us a systematic method to look for variational trial wave functions based on the functional form of the effective potential in the factorisation method of SQM.

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